Chapter 6
Review of Kriging Applications

This chapter will briefly treat three principal topics; applicability of kriging techniques, important elements that need to be addressed in kriging applications, and errors in measured data. Much of the information presented in this section has been gathered from other sections of this ETL and is presented collectively here. The items identified as important to kriging applications may be helpful in assessing kriging applications under review.

6-1. Applicability of Kriging

a. In the preceding sections of this ETL, the theory of kriging techniques has been summarized, and examples have been given to indicate the utility of kriging techniques in HTRW site investigations. The examples presented were selected so that kriging would provide satisfactory results or be applicable. Additionally, the examples were designed so that, for the purposes of demonstration, some sort of adjustment of the data was needed; that is, drift was removed or transformations were made.

b. Investigators are very likely to have data for which, although, in a strict sense, kriging may be applicable, results may be unsatisfactory. A good deal of fundamental information that may be used to establish how satisfactory application of kriging techniques might be has been presented in the preceding sections of this ETL. In particular, Chapter 4 includes a detailed discussion on variogram construction, the preliminary step in any kriging application, and systematically describes many decisions in this process that need attention. If the investigator cannot construct or otherwise obtain a variogram that has structure, then the results of a kriging application may not be satisfactory. Some additional discussion designed to guide investigators in evaluating the amount of data that may be required for kriging applications is presented in this section. This discussion will assume that the measured data are correct; a separate and brief discussion of measurement errors will also be presented in this section.

c. Many investigators will have a tendency to focus on the amount of measured data that is available as an initial consideration. It is important for the investigator to realize that decisions concerning the applicability of kriging techniques cannot be based simply on the amount of measured data. However, unless the investigator is presented with a reliable variogram, the amount and spatial distribution of measured data can be a constraint. If, for instance, the investigator has fewer than 25 measured values at optimal locations from the field, there may not be enough data to confidently estimate Gaussian variogram parameters, a smaller amount of measured data may be suitable for other variogram models.

d. The amount of data needed to apply kriging techniques is not easy to determine, but information in this ETL, especially in Chapter 4, and the literature cited can provide some guidance. Section 4-4 points out that a good minimum for the number of pairs of locations in each variogram lag is 30 and the American Society for Testing and Materials (Standard D 5922-96) has suggested that 20 may work well also. Most investigators would probably feel comfortable defining a Gaussian form (which, because it has more inflection, is more difficult to fit compared to the other standard variogram models) with 8 to 10 optimally located sample variogram points (enough points to define the nugget, two areas of curvature, and the sill). In this ideal case, about 25 measured values would be needed to fulfill the conservative minimum of 30 pairs per lag. In this case, the relatively few measured data points need to be systematically located so that the optimally located variogram points can be computed. If the measured data were not located systematically, as is usually the case, then more measured data would be needed.

e. Once sample variogram points meeting the required number of pairs of locations can be defined, the investigator needs to have a resulting variogram that has structure. The variogram, for instance, may simply exhibit noise about a horizontal line and have no structure. If measured data are clustered and the lags have been minimized to meet the required number of pairs of locations, the variogram may seem horizontal because it is dominated by small-scale effects in the clustered data. The investigator then has latitude to adjust the lags and attempt to balance the lag spacing and required number of pairs of locations, as described in section 4-4. However, the variogram could also seem horizontal because the actual sill is reached within a very small lag. If that lag is smaller than the minimum spacing of measured data, obtaining structure in the variogram would not be possible. If the investigator has a variogram with no structure, the measured data need to be considered independent, and kriging techniques, at the lag of the measured data, would be ineffective or at least offer little advantage over other interpolation techniques.

6-2. Important Elements of Kriging Applications

a. Many important elements of kriging applications have been discussed in this ETL. These discussions have been presented as a systematic and sequential method designed to provide guidance in kriging applications. Occasionally, an investigator will be presented with the results of a previous kriging application and will need to evaluate the application before deciding whether or not to use the results. This section presents a brief review of some important elements of kriging applications that such an investigator may use in that evaluation. For a more detailed discussion of important elements of geostatistical applications, the reader is referred to the American Society of Testing and Materials (Standard D 5549-94) for content of geostatistical investigations.

b. The presence of or lack of stationarity in the spatial mean needs to be demonstrated definitively. If the spatial mean is nonstationary, then drift is indicated and appropriate measures to establish stationarity, which are similar to the measures presented in section 4-3, need to be part of the application. In ideal situations, nonstationarity occurs as a gradual change. HTRW site investigations may present cases, especially when dealing with water- quality data in and around plumes, that have abrupt step-like changes at plume boundaries and do not appear as regional drift. In these cases the investigator needs to be aware that without knowledge of the plume boundaries, points from within the plume will be grouped with points from outside the plume in computing the sample variogram. The effect of this problem is minimized as long as the investigator can define lags that allow data points within the plume to be grouped together.

c. The construction of the variogram needs to be described. The description needs to address the number of pairs of locations in each variogram lag and to demonstrate that the variogram has structure. A plot of the variogram is helpful to demonstrate the presence or absence of structure. The variogram construction discussion also needs to establish the presence of or lack of isotropy. If anisotropy is present, its nature needs to be established, and it needs to be addressed by variogram adjustments similar to the adjustments presented in section 4-5*b*.

d. The variogram cross-validation statistics described in section 4-9 are useful and, if available, they can aid in the evaluation of a kriging application; authoritative and definitive kriging applications should include cross-validation. Cross-validation statistics need to conform to the guidelines discussed in section 4-9. Section 4-9*b* indicates that the cross-validation exercise needs to balance minimizing the kriging cross-validation errors with efforts to guard against bias. Also, as discussed in section 4-9*b*, if probabilistic statements are part of the kriging application, there needs to be some demonstration about the normality of the reduced kriging error such as the cross-validation probability plots included with the examples in Chapter 5.

e. Maps of the kriging estimates and standard deviations need to be presented or discussed. The maps of kriging estimates need to conform to any qualitative information about the information portrayed on the maps that is available to the investigator. The maps of kriged standard deviations can be used to determine where there are large areas of uncertainty in the kriging estimates.

f. Finally, the variogram and kriging algorithms are most useful as interpolation rather than extrapolation tools. Once the application extends to areas beyond the geographic extremes of the measured data, or perhaps those extremes plus the range, there needs to be some qualification of the area of extrapolation. For instance, in universal kriging, the practitioner would need to have some assurance that the conditions of drift defined in the study area continue into the area of extrapolation.

6-3. Errors in Measured Data

a. Data associated with HTRW site investigations have the same opportunities for errors that most investigations do. The errors may involve, among others, bias, inaccuracy, or lack of representativeness. The classical nature of these errors is described in EM 200-1-2, "Technical Project Planning," (U.S. Army Corps of Engineers 1995), which describes HTRW data-quality design.

b. The presence of contamination may complicate the function of errors in HTRW site investigations. Because these investigations often concern contamination, there can be large ranges of values for data involving contaminant concentrations, and these large ranges have a tendency to increase the incidence of data that may seem to be statistical outliers. Even more complicating is the presence of high concentrations of organic materials that may create challenging analytical problems in laboratory determinations that also may lead to reported values that seem to be statistical outliers. In either case, the kriging practitioner is likely to find that the apparent outliers have a strong effect on the results of the kriging application.

c. When HTRW site investigations find data that seem to be outliers, the data need to be very carefully evaluated before removal is seriously contemplated. Automated outlier detection tools, as suggested in section 4-8, may best be used to identify points that may be outliers and warrant further investigation. Often data that appear to be outliers may be the most important and meaningful data of all measurements. For example, in the first case described in the preceding paragraph, apparent outliers often are representative values. In the second case, the reported value may be an erroneous determination that has been affected by the extremely contaminated nature of the sample matrix. The investigator needs to either possess or have access to qualitative or institutional knowledge that will aid in outlier interpretation.